Introduction to Source Apportionment Methods

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Goal of Source Apportionment

- To determine contributions of various pollution sources to a location of interest (e.g.,outdoor, indoor, or personal exposure measurement)
- Approach is “receptor”-oriented

Common Apportionment Methods

1) Chemical Mass Balance (CMB) Modeling
2) Principal Component Analysis (PCA) [a type of factor analysis modeling]
3) Positive Matrix Factorization (PMF)

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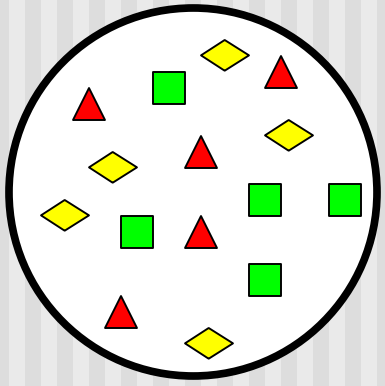
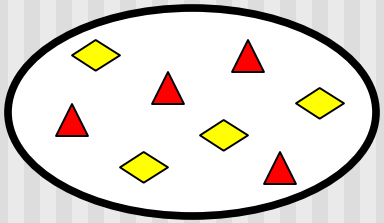
1) CMB Source Apportionment



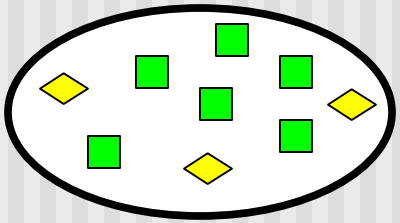
Sample

1) CMB Source Apportionment

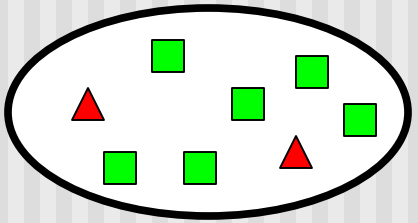
Known Source #1

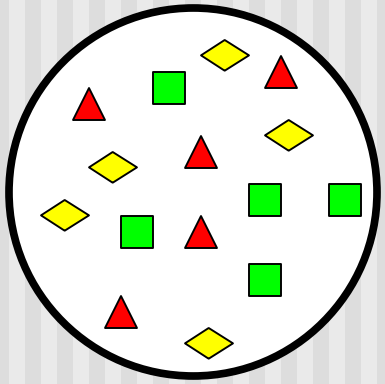


Known Source #2



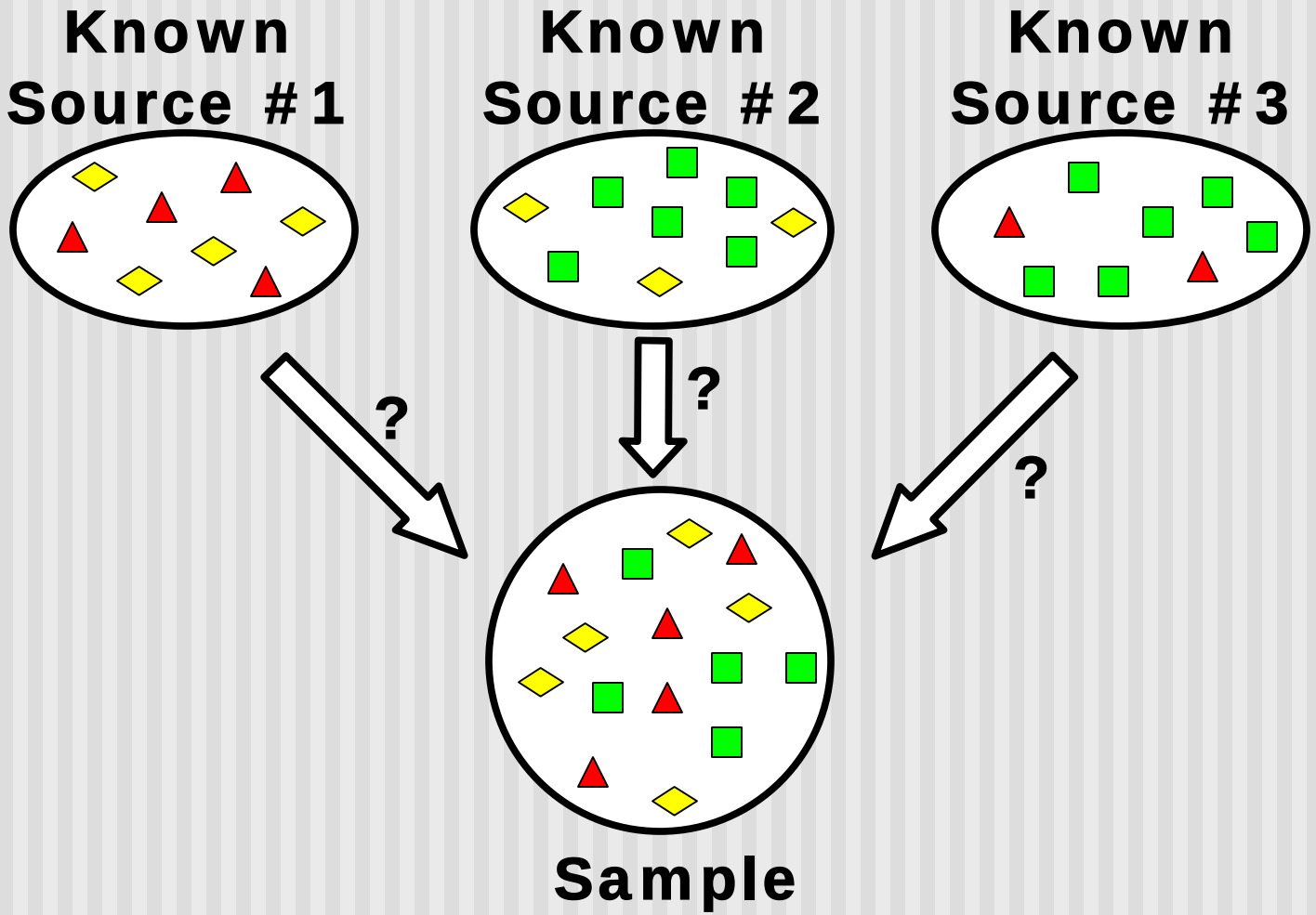
Known Source #3





Sample

1) CMB Source Apportionment



Limitations of CMB

- Must have complete emissions composition info. for each source
- Cannot have missing sources or missing data
- Tracer species must be nonreactive
- # of sources ? # of tracer species

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Pluses and Minuses of CMB

- Pluses
  - Can analyze single receptor samples
  - Apportionment results identify specific, well-known sources
- Minuses
  - Must learn to spot problems in model output (e.g., missing sources)
  - Cannot resolve sources that are collinear

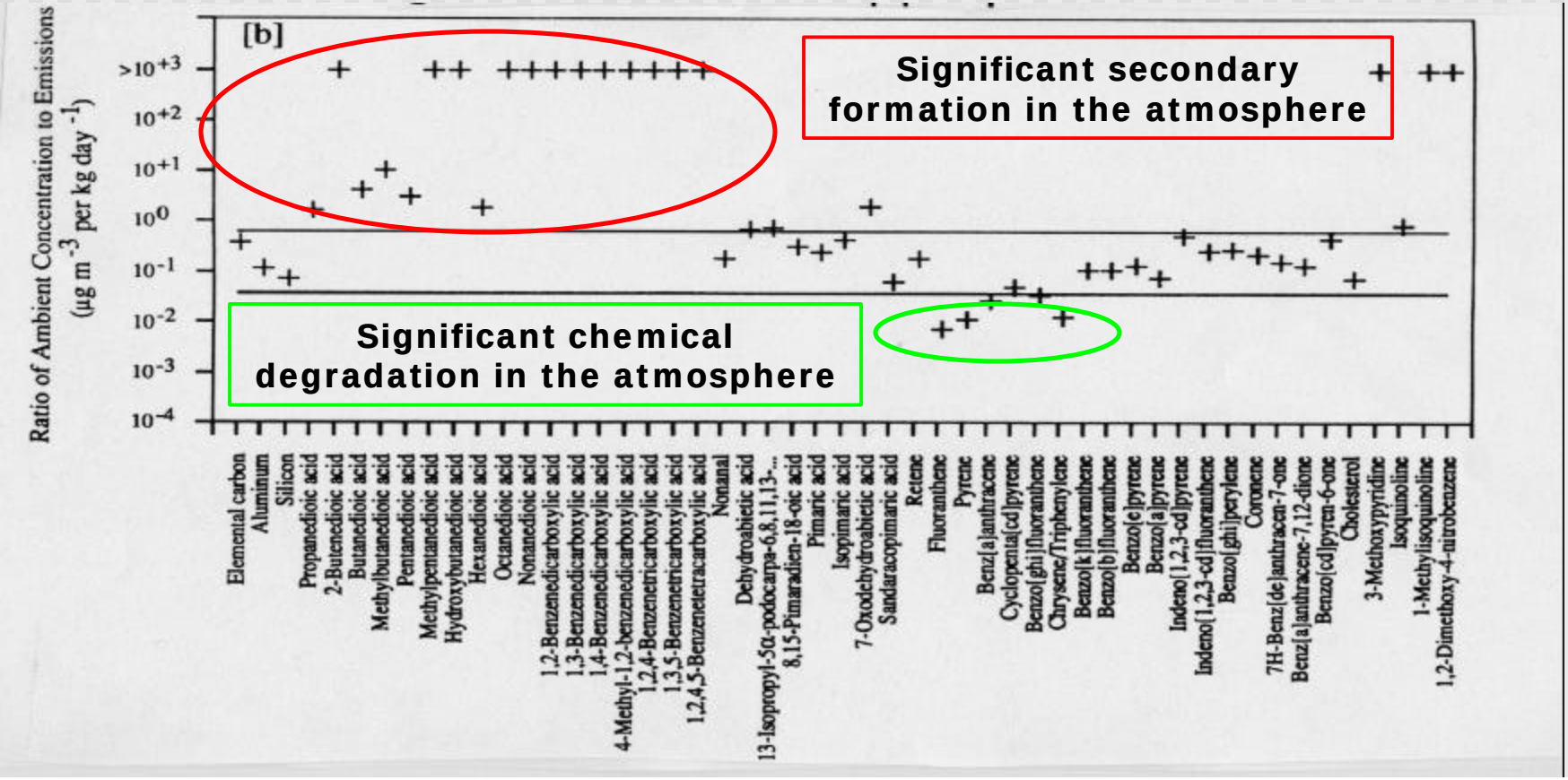
Recent Advances in CMB

- For PM source apportionment, trace metals and ionic species have traditionally been used as tracers
- More recent work has included stable organic aerosol species as tracers

CMB Modeling Example

[from JJ Schauer et al., Atm.Env. 30:3837 (1996)]

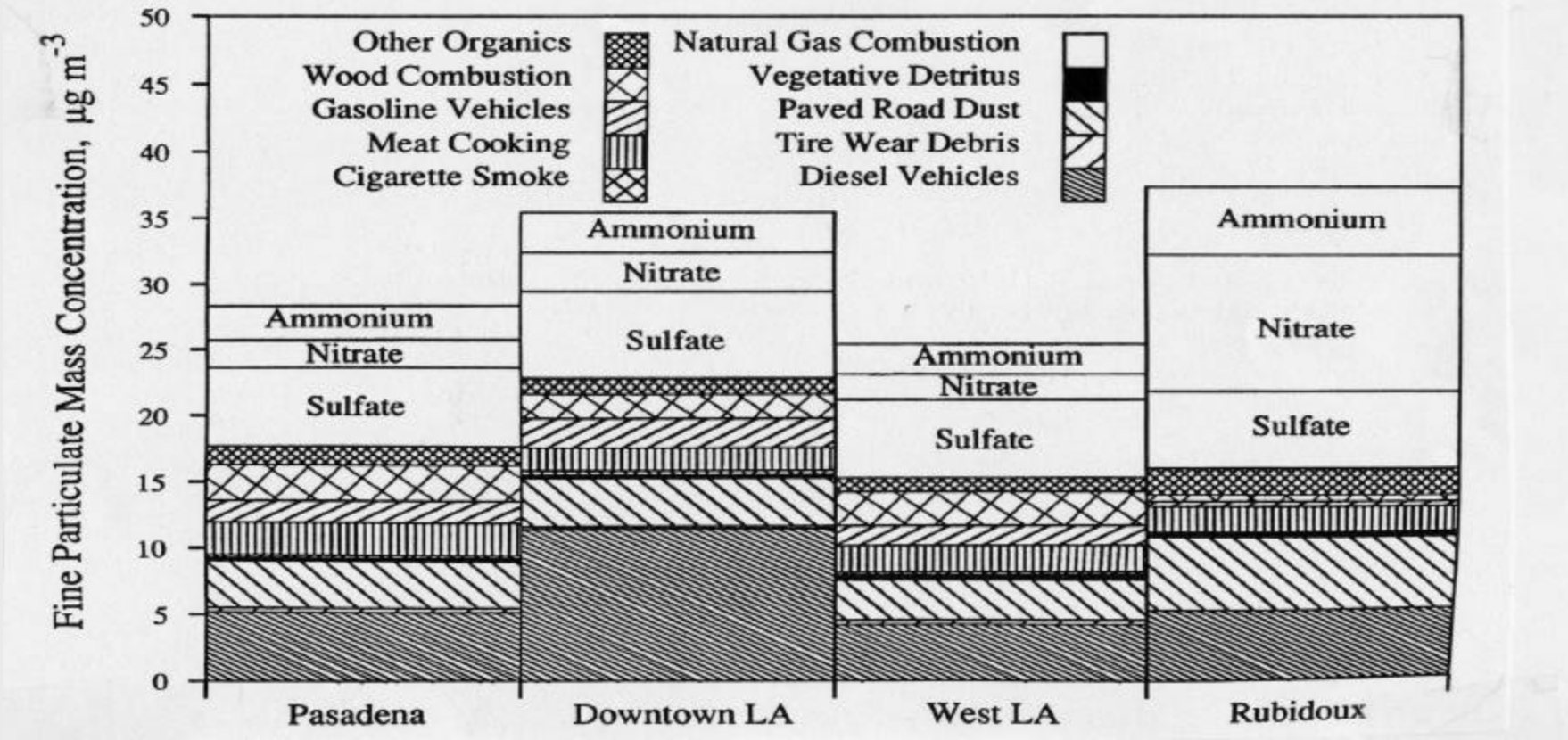
- Cass 'group first determined which organic compounds were stable enough tracers to be appropriate for CMB modeling



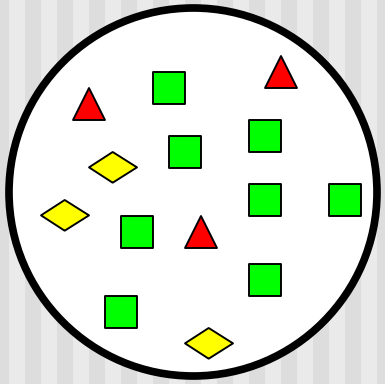
CMB Modeling Example (cont.)

[from JJ Schauer et al., Atm.Env. 30:3837 (1996)]

- CMB results apportioned total ambient PM2 concentrations among 9 primary sources

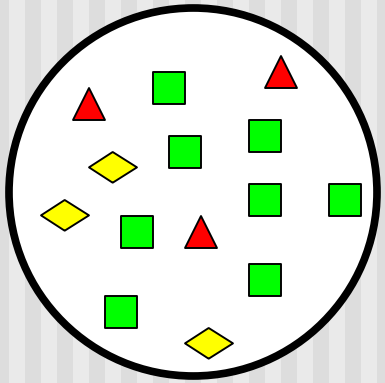


2) PCA Source Apportionment

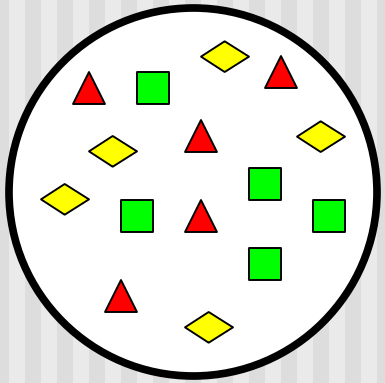


Sample

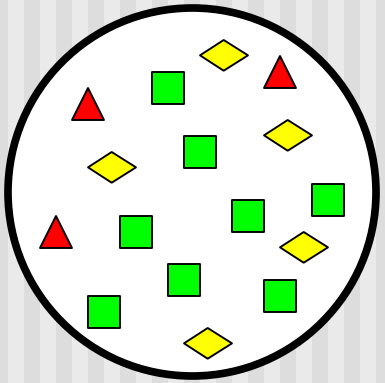
2) PCA Source Apportionment



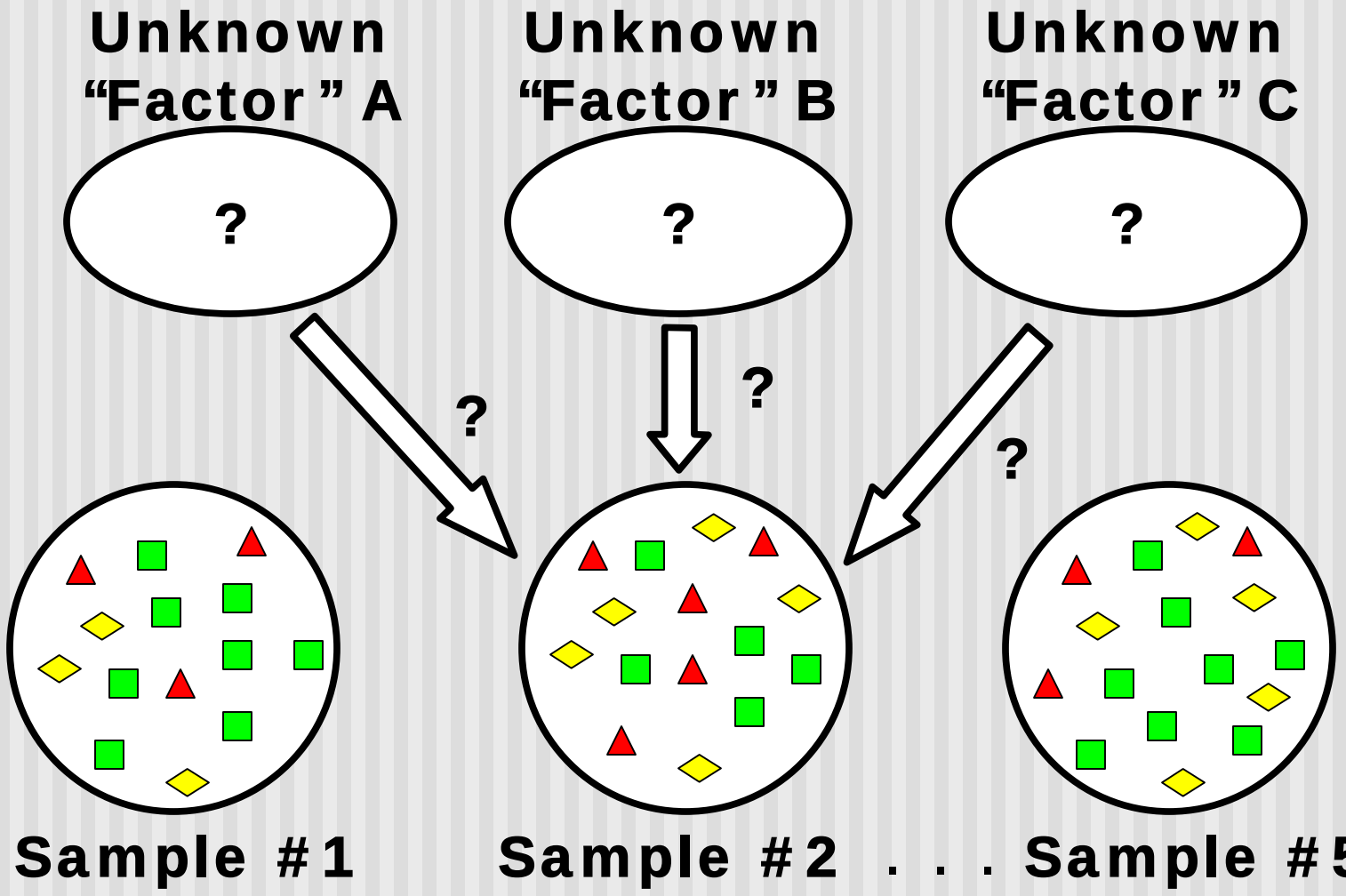
Sample #1



Sample #2 . . . Sample #50



2) PCA Source Apportionment



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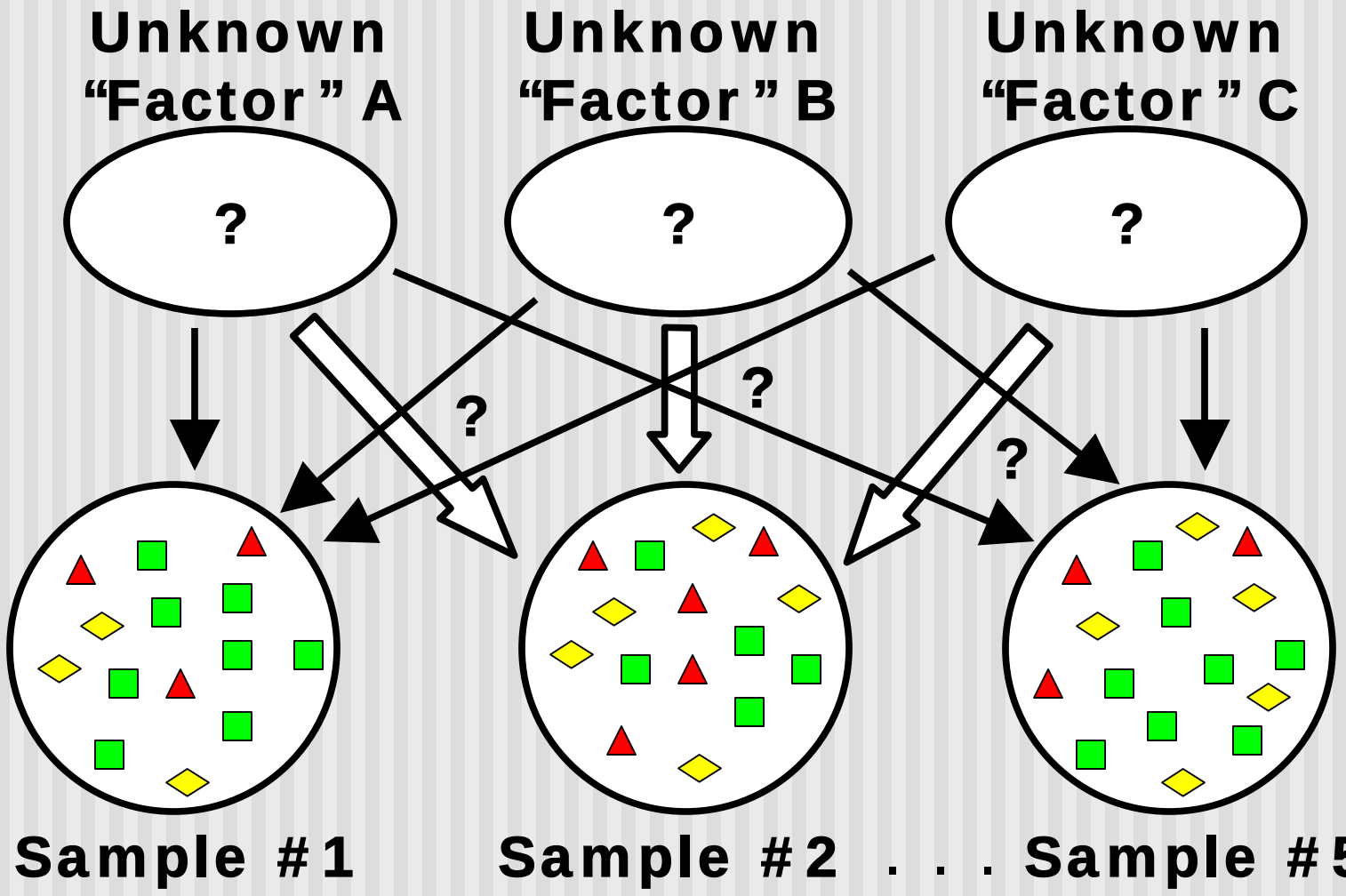


Limitations of PCA

- Need a large # of receptor samples
- Must determine how many "factors" to retain
- Must judge what source(s) is/are represented by each factor
- Can get negative values for chemical components, or factors that cannot clearly be connected to sources

Pluses and Minuses of PCA

- Pluses
  - Can be used without needing source emission compositions as inputs
  - Can help identify important missing sources
  - Often uses tracers that are somewhat reactive
- Minuses
  - Cannot weight solution to account for variations in uncertainties
  - A large number of solutions can be obtained; even with Varimax rotation, cannot be sure that the optimal solution has been found

PCA Modeling Example

[from RD Edwards et al., Atm.Env. 35:4829 (2001)]

Samples: 111, from nonsmoking residences

Tracers: 22 Volatile Organic Compounds

Number of "factors" retained: 6

Factor assignments:

1 = indoor cleaning products

2 = traffic emissions

3 = long range transport

4 = bldg. emissions, mold/fungal growth

5 = carpets and/or adhesives

6 = more mold due to less cleaning

3) Positive Matrix Factorization

- PMF modeling is a recent advance in source apportionment modeling
- Like PCA, is a multivariate modeling technique that does not need source compositions as inputs
- Like PCA, simultaneously identifies "factors" and their contributions to a receptor sample

Differences between PCA and PMF

- PMF constrains solutions to be > 0 (so "factors" do not have negative chemical components)
- PMF can account for uncertainties in the input measurements
- PMF can handle missing or below-detection-limit input data

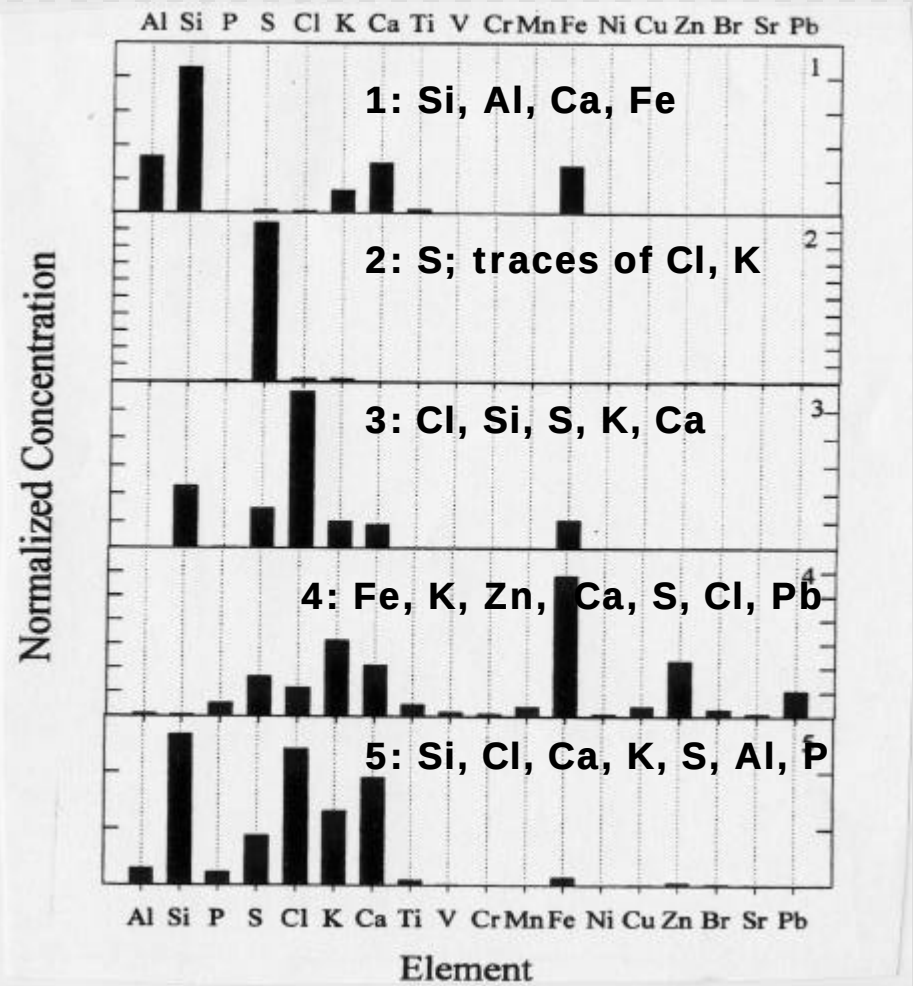
PMF Modeling Example

[from E Yakovleva et al., ES&T 33:3645 (1999)]

Samples: 178 personal exposure measurements

Tracers: 18 trace elements from PM10 samples

No. of "factors" retained: 5



PMF Modeling Example

[from E Yakovleva et al., ES&T 33:3645 (1999)]

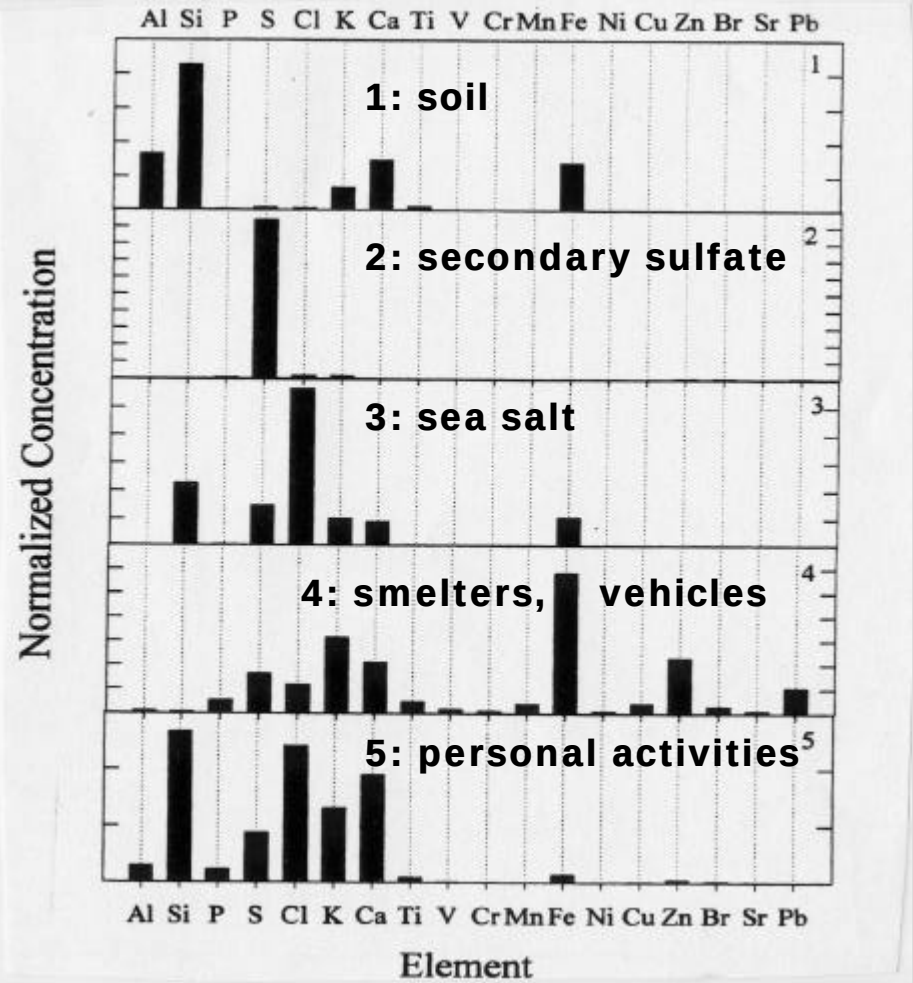
Samples: 178 personal exposure measurements

Tracers: 18 trace elements from PM10 samples

No. of "factors" retained: 5

Factor assignments:

- 1 = soil
- 2 = secondary sulfate
- 3 = sea salt
- 4 = smelters and motor vehicles
- 5 = personal activities



PMF Modeling Example (cont.)

[from E Yakovleva et al., ES&T 33:3645 (1999)]

- By regressing PM concentrations against PMF factors, source contributions can be found

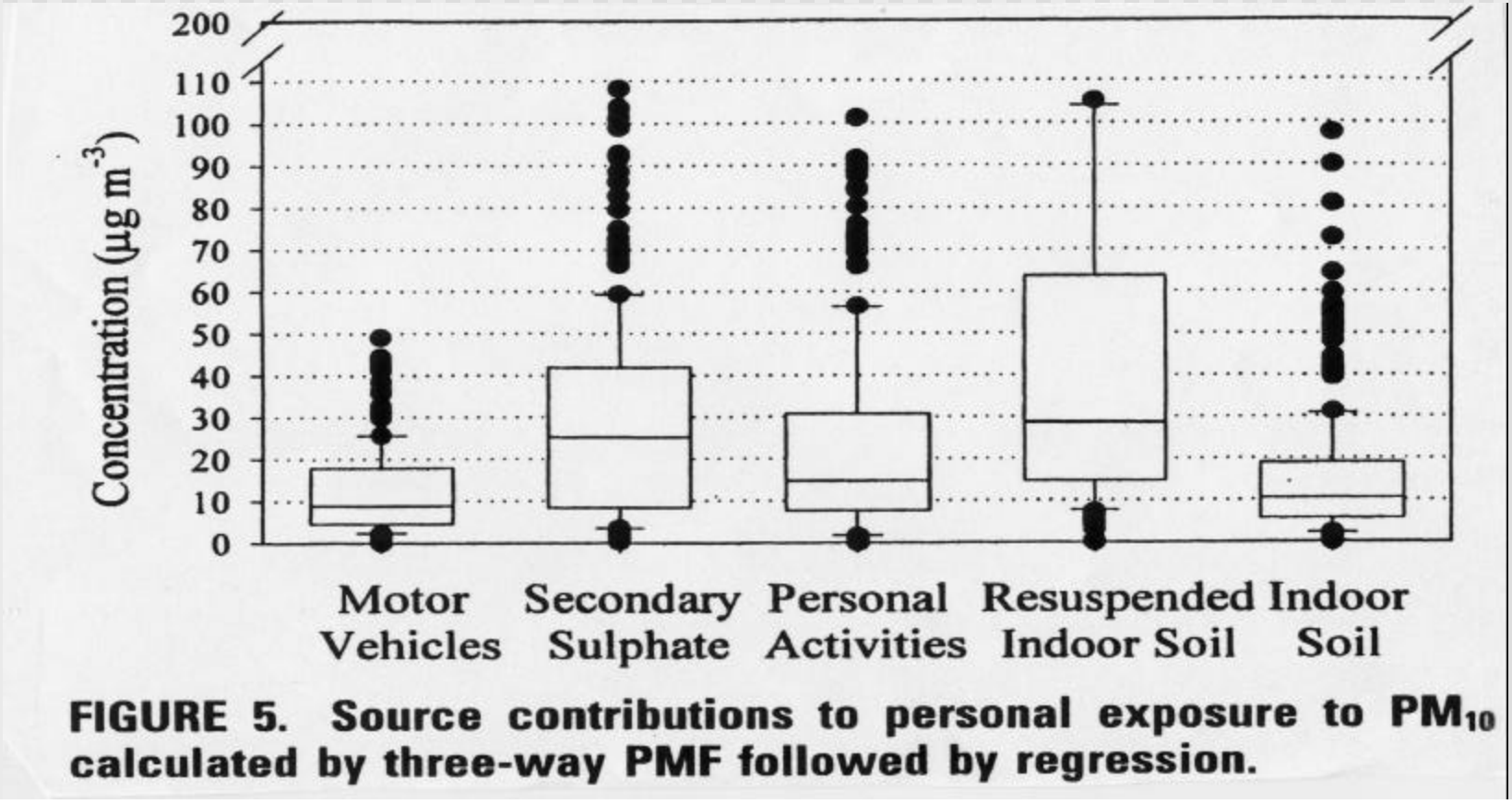


FIGURE 5. Source contributions to personal exposure to PM_{10} calculated by three-way PMF followed by regression.

Summary of 3 Methods

	CMB	PCA	PMF
Can run without source compositions as inputs?		?	?
Can run with a small # of receptor samples?	?		
Can reactive compounds be used as tracers?	?	?	?
Can include measurement uncertainties?	?		?
Can handle missing data?			?
Can handle below-detection-limit data?	?		?
Must determine optimal # of "factors"?		?	?
Must interpret "factors" to identify sources?		?	?
Must determine if there are missing sources?	?		
May encounter problems with collinearity?	?	?	?